Flucythrinate

70124-77-5 | DTXSID0022301

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.00e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 4.08e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

Image not found
1,2,3,4,6-Pentachloronaphthalene
Measured: 8.70e-09
Predicted: 1.71e-06

Image not found
2,3',4-Trichlorodiphenyl ether
Measured: 1.20e-09
Predicted: 1.55e-04

Image not found
Hexazinone
Measured: 1.50e-09
Predicted: 4.91e-07

Image not found
Pentane, 2,3,3-trimethyl-
Measured: 7.59e-10
Predicted: 29.7